ENERGY ERROR ESTIMATE FOR COUPLED-CLUSTER EXCITED STATES

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In our recent work [1], the nonlinear equations of the single-reference Coupled-Cluster method have been analysed using topological degree theory. This generalizes previous work based on (local) strong monotonicity [2]. We have established existence results and qualitative information about the solutions of these equations that also sheds light on some of the numerically observed behavior. In particular, to investigate truncation schemes within the Coupled-Cluster method, we have utilized the Kowalski-Piecuch homotopy [3]. In this setting, we have derived an energy error bound for approximate eigenstates of the Schrödinger equation, i.e., for both ground and excited states.

REFERENCES

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